Robust and efficient solvers for large and indefinite linear systems

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In many ComPASS EM applications, solving linear systems is the "memory" bottleneck;

$$Ax = b,$$

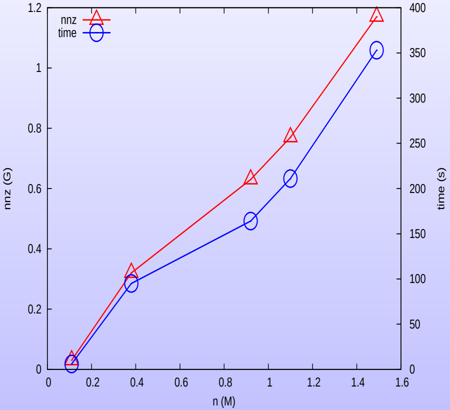
where A is

- large and sparse
  - direct methods are robust, but require infeasibly large memory.
- ill-conditioned and highly-indefinite
  - preconditioned iterative methods require less memory, but suffer from slow or no convergence.

Hybrid methods have the potential of balancing memory and time;

- techniques from direct methods are used to transform the original system into a "smaller" system, which is "easier" to solve by iterative methods.

Direct method: SuperLU_DIST with MeTiS

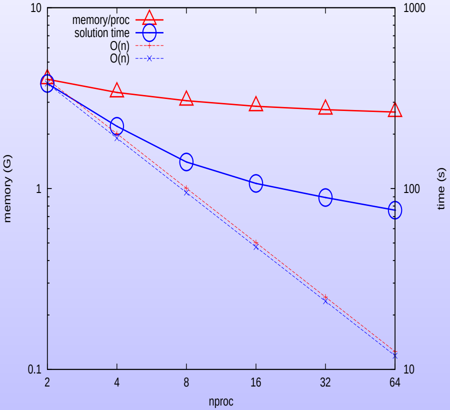


	n (M)	nnz (G)	fill-ratio	time (s)
dds	0.02	0.02	4	6
tdr108	0.11	0.03	18	6
quad	0.38	0.32	21	95
tdr158	0.92	0.63	17	164
tdr190	1.10	0.77	18	211
tdr256	1.49	1.17	20	353

two processes running on two nodes of Franklin.

- large amount of fill: **tdr256k** could not be solved on one node (which has 7.38GB of memory).

Direct method: SuperLU_DIST with MeTiS

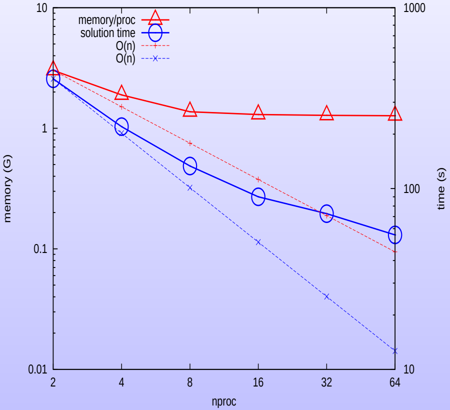


nproc	mem (GB)	time (s)	speed up
2	4.02	380.95	1.00
4	3.40	221.06	1.72
8	3.06	140.26	2.72
16	2.85	102.81	3.71
32	2.73	89.18	4.27
64	2.65	75.97	5.01

tdr256k performance profiled using Craypat on Franklin.

- memory requirement scales poorly with the number of processors.
  - each process required an explicit use of entire memory on a node.

Direct method: SuperLU_DIST with ParMeTiS



nproc	mem (GB)	time (s)	speed up
2	3.02	404.42	1.00
4	1.89	219.98	1.83
8	1.37	133.26	3.03
16	1.30	90.00	4.49
32	1.28	72.65	5.57
64	1.27	55.43	7.30

tdr256k performance profiled using Craypat on Franklin.

- parallel permutation and symbolic factorization improve scalability.
- memory requirement can still be the bottleneck.

Preconditioned iterative method: Phidal [Henon and Saad '06]

- GMRES(100) to achieve $\|b - Ax\|_2 / \|b\|_2 \leq 10^{-12}$ on one core of Franklin.

drop tol.	fill-ratio	itrs	ptime	stime	ttime
SuperLU	17.52	$--$	7.54	0.39	7.93
10^{-5}	14.85	17	10.79	2.64	13.47
10^{-4}	12.84	> 1000	7.60	$--$	$--$

$105,386 \times 105,386$ **tdr108k**, times are in seconds.

drop tol.	fill-ratio	itrs	ptime	stime	ttime
SuperLU	20.53	$--$	167.57	2.03	169.60
10^{-4}	19.95	50	732.70	77.07	809.77
10^{-3}	19.91	> 1000	743.04	$--$	$--$

$380,698 \times 380,698$ **dds-quad**, times are in seconds.

- no convergence with a relatively large number of nonzeros.
- larger system often requires a larger fill-ratio for convergence.

Hybrid method: Schur complement method

Step 1: Reorder A into a 2×2 block system of the form

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

where

- A_{11} is $n_1 \times n_1$ block-diagonal, and A_{22} is $n_2 \times n_2$.
- A_{11} is typically referred to as the *interior domains*, A_{22} is called the *separators*, and A_{21} and A_{12} are the *interfaces* between A_{11} and A_{22}.
- Existing software like ParMeTiS, PT-SCOTCH, or HID can be used to create the block structure.

Hybrid method: Schur complement method

Step 1: With a block Gaussian elimination, the 2×2 block system becomes

$$\begin{pmatrix} A_{11} & A_{12} \\ 0 & S \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} I & 0 \\ -A_{21}A_{11}^{-1} & I \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \end{pmatrix},$$

where $S = A_{22} - A_{21}A_{11}^{-1}A_{12}$ is called the Schur complement.

Hence, the solution to the linear system is given by

- $Sx_2 = b_2 - A_{21}A_{11}^{-1}b_1$ (**Steps 2** and **3**), and
- $A_{11}x_1 = b_1 - A_{12}x_2$ (**Step 4**).

Hybrid method: Schur complement method
Step 2: Solve the system of interior domains;

$$A_{11} z_1 = b_1$$

for z_1, based on an exact LU factorization of A_{11},

$$A_{11} \rightarrow L_1 U_1,$$

where L_1 is lower-triangular and U_1 is upper-triangular.

- Each diagonal block can be factored and solved independently using software like SuperLU_DIST.
- Appropriate scaling and permutation are applied to enhance numerical stability and preserve sparsity.

Hybrid method: Schur complement method
Step 3: Approximately solve

$$Sx_2 = \widehat{b}_2$$

for x_2, where S is the **Schur complement**, and $\widehat{b}_2 = b_2 - A_{21}z_1$.

Krylov method (e.g. GMRES) is used with a preconditioner based on an incomplete factorization of S:

$$\begin{cases} S &= \widetilde{S} + E_S, \\ \widetilde{S} &= \widetilde{L}_2\widetilde{U}_2 + E_{LU}, \end{cases}$$

where

- E_S and E_{LU} are error matrices.
- Sparsity of $\widetilde{S}$, $\widetilde{L}_2$, and $\widetilde{U}_2$ is enforced by discarding small nonzeros.
- S is accessed only through matrix-vector multiply.

Hybrid method: Schur complement method

Step 4: Solve the system of interior domains;

$$A_{11}x_1 = \widehat{b}_1,$$

where $\widehat{b}_1 = b_1 - A_{12}x_2$, and the factorization of A_{11} from **Step 2** is used.

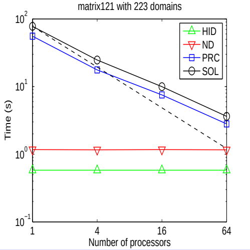
Our **motivations** for focusing on this hybrid method is

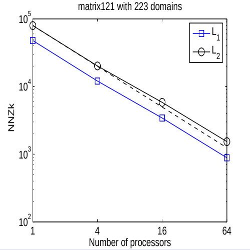
- memory requirement: fill is restricted within
  - "small" diagonal blocks of L_1 and U_1, and
  - $\widetilde{S}$, $\widetilde{L}_2$, and $\widetilde{U}_2$, whose "sparsity" can be enforced.
- conditioning: in comparison to A,
  - S is smaller in its dimension, and
  - S often has more favorable eigenvalue distribution.

  The linear system with S is expected to be "easier" to solve using a preconditioned iterative method
- parallelism: interior domains are solved independently.

HIPS (Hybrid Iterative Parallel Solver):

- Developed by Pascal Henon (INRIA) and Yousef Saad (UM), 2008.
- Based on HID to achieve scalability on a parallel machine.





- Current limitations:
  - Number of processors cannot exceed the number of interior domains.
  - Fill in ILU($\widetilde{S}$) is restricted within the "level-1" blocks of A_{22}.

  To run on many processors, many interior domains are needed, which results in slow or no convergence
  - large Schur complement and poor preconditioner (fill is restricted within small blocks).

Results of HIPS

tol	dom	n_2	nnz	fill-fact	itrs	ptime	stime	ttime
direct	1	$--$	13M	16.8	$--$	3.22	0.14	3.41
10^{-4}	2	54	13M	16.7	4	3.77	0.64	4.47
	4	238	13M	16.3	6	3.78	0.80	4.64
	8	1774	10M	13.5	24	3.35	2.14	5.57
	15	3056	9M	12.1	56	3.72	4.65	8.44
	32	6091	8M	10.1	680	4.76	58.44	63.31
	61	9556	7M	8.8	> 2000	5.35	$--$	$--$
10^{-6}	32	6091	8M	11.0	85	9.12	7.85	17.08
	61	9556	7M	9.8	> 2000	8.66	$--$	$--$

$105,386 \times 105,386$ **tdr108k** with $\mathrm{nnz}(A) = 804,301$.

- Large number of domains is needed to reduce memory cost.
- GMRES(100) does not converge with a large number of domains.
- Larger system requires a smaller number of domains for convergence, i.e., for **tdr256k**, HIPS did not converge with 4 interior domains.

New implementation of the hybrid method, whose performance is better than HIPS. Our goals are to

- improve numerical stability,
- solve each interior domain with multiple processors, and
- implement our own parallel ILU.

Implementation approach:
we rely on existing software (performance, development time, etc.);

- **Step 1**: initial partitioning is computed by HID.
- **Step 2**: system of interior domains is solved using SuperLU_DIST.
- **Step 3**: drop tolerance σ_1 enforces sparsity of $\widetilde{S}$, and drop tolerance σ_2 enforces sparsity of $\widetilde{L}_2$ and $\widetilde{U}_2$.

	σ_1	σ_2	ILU/LU	Solve
(1)	zero	zero	SLU	SLU
(2)	nonzero	zero	SLU	PETSc
(3)	zero	nonzero	PHIDAL	HIPS
(4)	nonzero	nonzero	PHIDAL	PETSc

Four configurations to solve the Schur complement.

- **Step 4**: system of interior domains is solved by SuperLU_DIST, using their LU factorizations from Step 2.

Preliminary results of new implementation

	σ_1	σ_2	nnz	fill-ratio	itrs	ptime	stime	ttime
(1)	0.0	0.0	5.5M	4.0	−−	3.02	0.05	3.07
(4)	10^{-4}	10^{-4}	0.6M	0.5	300	1.50	8.47	9.97

$17,732 \times 17,732$ **dds** with 147 domains, times are in seconds.

	σ_1	σ_2	nnz	fill-ratio	itrs	ptime	stime	ttime
(1)	0.0	0.0	24M	16.8	−−	18.53	0.51	19.04
(4)	10^{-2}	10^{-4}	22M	15.6	64	71.92	43.78	115.70

$105,386 \times 105,386$ **tdr108k** with 468 domains, times are in seconds.

- GMRES(100) converged with the new implementation.
  - HIPS did not converge for **dds** and **tdr108k** with 25 and 61 domains, respectively.
- For a large system, Phidal and SuperILU require large amount of fill.

Preliminary results of new implementation

		$\mathrm{LU}(A_{11})$		$\mathrm{ILU}(\widetilde{S})$	
n_1	n_2	nnz	ratio	nnz	ratio
79,278	26,108	1.4M	3.2	20.6M	125.1

memory requirements for **tdr108k**.

$\mathrm{LU}(A_{11})$	$\mathrm{Comp}(\widetilde{S})$	$\mathrm{ILU}(\widetilde{S})$	Solve	Total
1.16	6.93	63.83	43.78	115.70

time requirements in seconds for **tdr108k**.

- $\mathrm{ILU}(\widetilde{S})$ is the memory bottleneck.
- time for $\mathrm{ILU}(\widetilde{S})$ and Solve is large due to large amount of fill.
- $\mathrm{Comp}(\widetilde{S})$ can be the bottleneck for a large matrix.

Current work:

- improving the convergence rate for solving the system of Schur complement
  - improving the quality of preconditioner, i.e., drop tolerance based ILU.
  - controlling the conditioning of the Schur complement.
- improving the time efficiency for computing Schur complement.
  - symbolic factorization to take advantage of sparisity.
- developing parallel implementation.
- conducting further experimentation.

Extra slides

Schur complement computation:

S is computed domain-by-domain,

$$
\begin{aligned}
& A_{22} - A_{21} A_{11}^{-1} A_{12} \\
&= A_{22} - \begin{pmatrix} A_{21}^{(1)} & A_{21}^{(2)} & \dots & A_{21}^{(\ell)} \end{pmatrix} \begin{pmatrix} A_{11}^{(1)} & & & \\ & A_{11}^{(2)} & & \\ & & \ddots & \\ & & & A_{11}^{(\ell)} \end{pmatrix}^{-1} \begin{pmatrix} A_{12}^{(1)} \\ A_{12}^{(2)} \\ \vdots \\ A_{12}^{(\ell)} \end{pmatrix} \\
&= A_{22} - \sum_{i=1}^{\ell} A_{21}^{(i)} B_i^{-1} A_{12}^{(i)}.
\end{aligned}
$$

- each $A_{11}^{(i)}$ is scaled and permuted for numerical stability.
- each $A_{21}^{(i)}$ and $A_{12}^{(i)}$ are stored in the CSR and CSC formats.
- S is formed by k columns at a time and stored in the CSC format.

For a symmetric A,

Schur complement is computed as

$$
\begin{aligned}
& A_{22} - \textstyle\sum_{i=1}^{\ell} A_{21}^{(i)} A_{(11)}^{(i)-1} A_{12}^{(i)} \\
&= A_{22} - \textstyle\sum_{i=1}^{\ell} (L_i^{-1} A_{12}^{(i)})^T (L_i^{-1} A_{12}^{(i)}) \\
&= A_{22} - \textstyle\sum_{i=1}^{\ell} W_i^T W_i
\end{aligned}
$$

- eliminates one triangular solve
  - computation time can be reduced to about half.
- requires memory to store W_i
  - only one W_i needs to be stored at a time.
- takes advantage of sparsity of W_i
  - sparsity of W_i can be enforced.

Preprocessing:
S is preprocessed to minimize possibility of a singular $\widetilde{S}$:

$$S = P_r D_r S D_c,$$

- P_r is a row permutation to move large elements to the diagonals.
- D_c and D_r are column and row scaling matrices, respectively such that S has unit diagonals.
- this preprocess is efficiently applied since S is stored in CSC.

The subroutine **mc64ad** developed by Iain Duff is used.

Compute ILU of $\widetilde{S}$:

- enforce sparsity of $\widetilde{S}$.
  - discard nonzeros of S with magnitudes less than a drop tolerance σ_1.
- compute LU or ILU factorization of $\widetilde{S}$ using SuperLU or Phidal.
  - SuperILU based on level computation after the symbolic factorization of each columns of $\widetilde{L}_2$ and $\widetilde{U}_2$.
- free memory used to store $\widetilde{S}$.

	nnz	fill-ratio	itrs	ptime	stime	ttime
Direct	287M	19.51	−−	579.53	1.66	581.19
Phidal(10^{-4})	277M	18.92	59	2,026.35	61.88	2,088.23
SuperILU(2)	239M	15.28	4	802.88	9.52	812.40

$380,698 \times 380,698$ **dds-quad** with 284 domains.

- for **dds-quad**, HIPS did not converge for 8 domains.